Cyclohexanone, 2,2-dimethyl-

Other names:	2,2-Dimethyl-1-cyclohexanone
	2,2-Dimethylcyclohexanone
	6,6-Dimethylcyclohexanone
Inchi:	InChI=1S/C8H14O/c1-8(2)6-4-3-5-7(8)9/h3-6H2,1-2H3
InchiKey:	KNSPBSQWRKKAPI-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CC1(C)CCCCC1=O
Mol. weight [g/mol]:	126.20
CAS:	1193-47-1

Physical Properties

Property code	Value	Unit	Source
gf	-87.15	kJ/mol	Joback Method
hf	-276.59	kJ/mol	Joback Method
hfus	1.52	kJ/mol	Joback Method
hvap	36.93	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.156		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	470.05	K	Joback Method
tc	700.41	K	Joback Method
tf	279.42	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.36	J/mol×K	470.05	Joback Method
cpg	264.46	J/mol×K	508.44	Joback Method
cpg	280.52	J/mol×K	546.84	Joback Method
cpg	295.62	J/mol×K	585.23	Joback Method
cpg	309.86	J/mol×K	623.62	Joback Method
cpg	323.33	J/mol×K	662.01	Joback Method

cpg	336.13	J/mol×K	700.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42371e+01
Coeff. B	-3.68015e+03
Coeff. C	-6.49020e+01
Temperature range (K), min.	328.72
Temperature range (K), max.	477.21

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1193471&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume